

43-03

FILE 'HOME' ENTERED AT 12:32:06 ON 03 JUN 2003

=> file reg	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 12:32:15 ON 03 JUN 2003  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 1 JUN 2003 HIGHEST RN 523977-56-2  
DICTIONARY FILE UPDATES: 1 JUN 2003 HIGHEST RN 523977-56-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

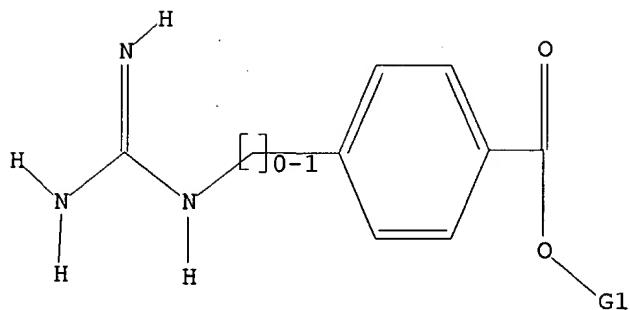
Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>  
Uploading 09975136 before allowance.str

L1 STRUCTURE UPLOADED

=> id l1  
COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID  
The query entered contains both search terms created by structure-building or screen commands and text search terms. L#s created via the STRUCTURE or SCREEN commands must be searched in the structures files separately from text terms or profiles. The L# answer sets from structure searches can be used in crossover searches and can be combined with text terms.

=> d l1  
L1 HAS NO ANSWERS  
L1 STR



G1 H,Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam

SAMPLE SEARCH INITIATED 12:32:49 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 208 TO ITERATE

100.0% PROCESSED 208 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

50 ANSWERS

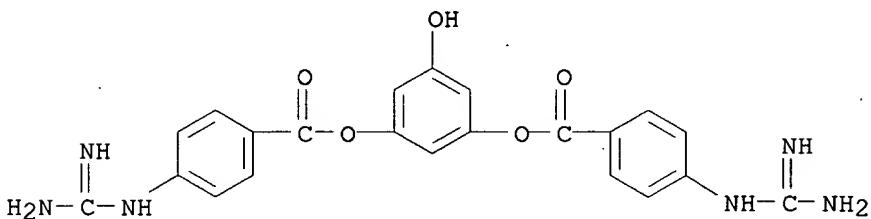
FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 3295 TO 5025  
PROJECTED ANSWERS: 1047 TO 2113

L2 50 SEA SSS SAM L1

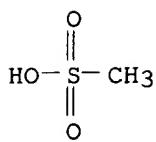
=> d scan

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 5-hydroxy-1,3-phenylene ester,  
dimethanesulfonate (salt) (9CI)  
MF C22 H20 N6 O5 . 2 C H4 O3 S

CM 1

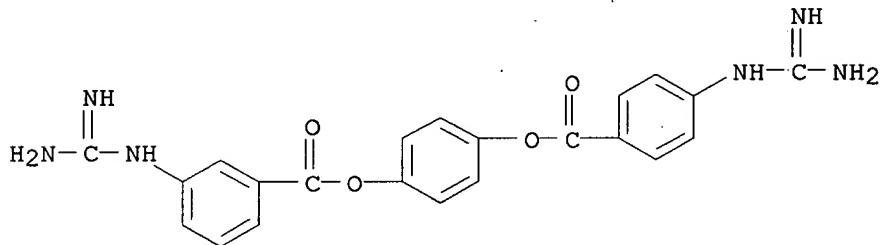


CM 2



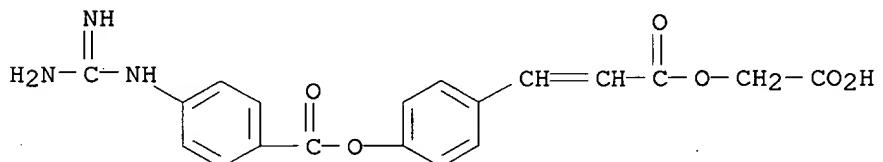
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 3-[(aminoiminomethyl)amino]-, 4-[[4-  
     [(aminoiminomethyl)amino]benzoyl]oxy]phenyl ester (9CI)  
 MF C22 H20 N6 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-,  
 4-[3-(carboxymethoxy)-3-oxo-1-  
     propenyl]phenyl ester (9CI)  
 MF C19 H17 N3 O6  
 CI COM



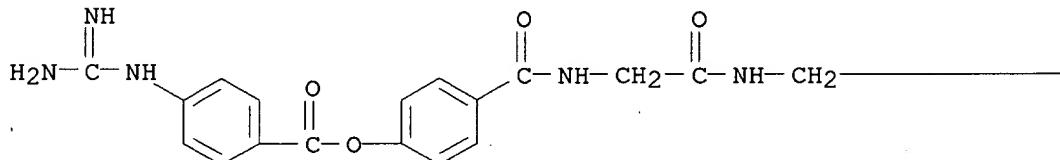
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Poly(oxy-1,2-ethanediyl), .alpha.-[2-[[[[4-[[

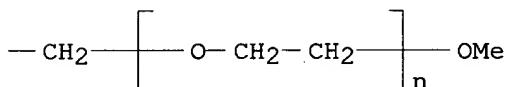
[ (aminoiminomethyl)amino]benzoyl]oxy]benzoyl]amino]acetyl]amino]ethyl]-  
omega.-methoxy-, monomethanesulfonate (9CI)  
MF (C<sub>2</sub> H<sub>4</sub> O)<sub>n</sub> C<sub>20</sub> H<sub>23</sub> N<sub>5</sub> O<sub>5</sub> . C H<sub>4</sub> O<sub>3</sub> S

CM 1

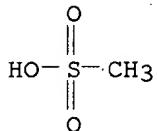
PAGE 1-A



PAGE 1-B

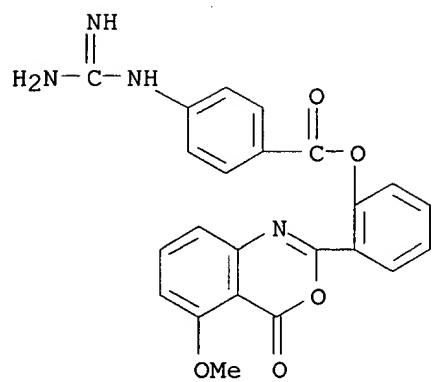


CM 2

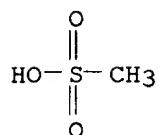


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[ (aminoiminomethyl)amino]-, 2-(5-methoxy-4-oxo-4H-3,1-  
benzoxazin-2-yl)phenyl ester, monomethanesulfonate (9CI)  
MF C<sub>23</sub> H<sub>18</sub> N<sub>4</sub> O<sub>5</sub> . C H<sub>4</sub> O<sub>3</sub> S

CM 1

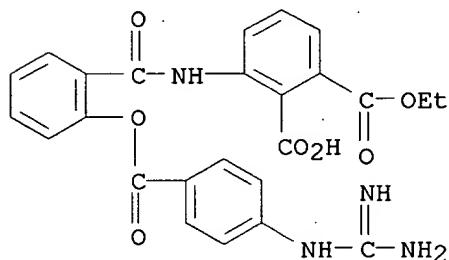


CM 2

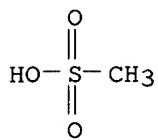


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 1,2-Benzenedicarboxylic acid,  
 3-[2-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]benzoyl]amino]-, 1-ethyl ester, monomethanesulfonate (9CI)  
 MF C25 H22 N4 O7 . C H4 O3 S

CM 1



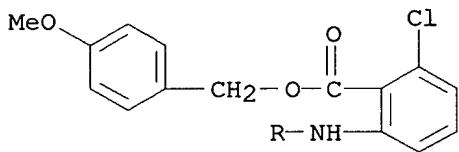
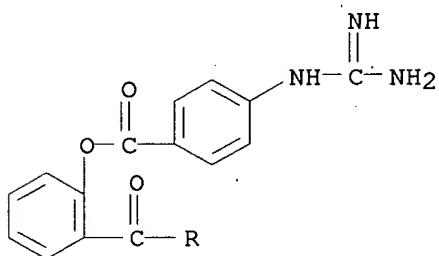
CM 2



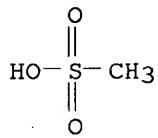
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):30

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid,  
 2-[[2-[(4-[(aminoiminomethyl)amino]benzoyl]oxy]benzoyl]amino  
 ]-6-chloro-, (4-methoxyphenyl)methyl ester, monomethanesulfonate (9CI)  
 MF C30 H25 Cl N4 O6 . C H4 O3 S

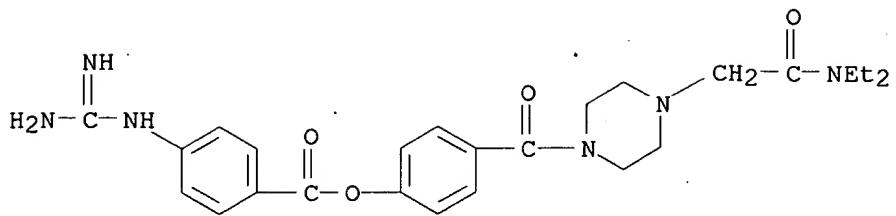
CM 1



CM 2



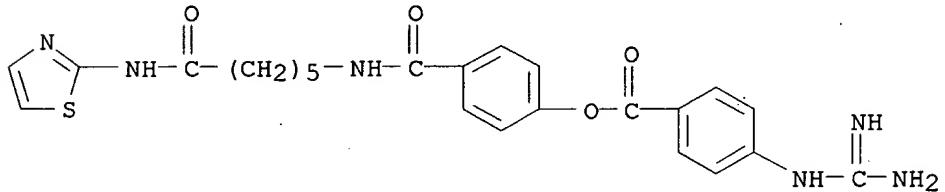
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[4-[2-(diethylamino)-2-  
 oxoethyl]-1-piperazinyl]carbonyl]phenyl ester (9CI)  
 MF C25 H32 N6 O4  
 CI COM



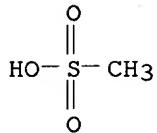
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[[6-oxo-6-(2-thiazolylamino)hexyl]amino]carbonyl]phenyl ester, monomethanesulfonate (9CI)  
 MF C24 H26 N6 O4 S . C H4 O3 S

CM 1

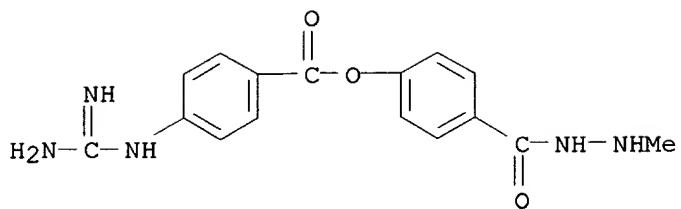


CM 2

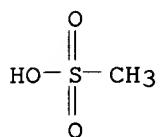


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[(2-methylhydrazino)carbonyl]phenyl ester, monomethanesulfonate (9CI)  
 MF C16 H17 N5 O3 . C H4 O3 S

CM 1

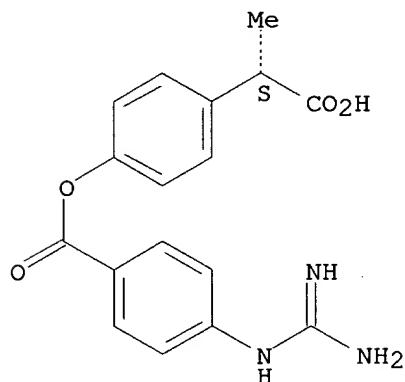


CM 2



L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzeneacetic acid, 4-[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, (S)- (9CI)  
 MF C17 H17 N3 O4  
 CI COM

Absolute stereochemistry.

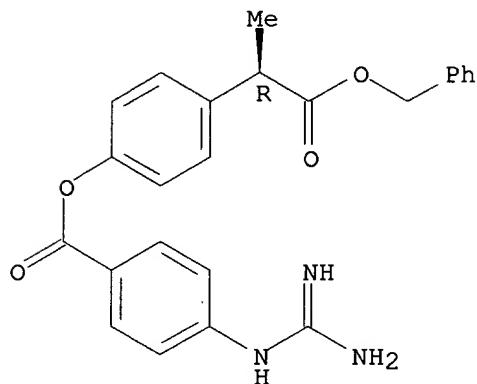


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

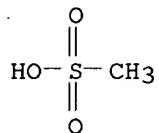
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzeneacetic acid, 4-[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, phenylmethyl ester, (R)-, monomethanesulfonate (9CI)  
 MF C24 H23 N3 O4 . C H4 O3 S

CM 1

Absolute stereochemistry.

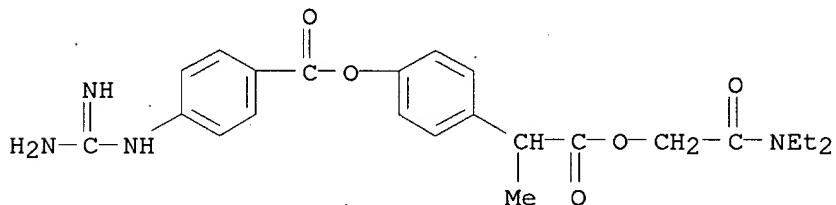


CM 2

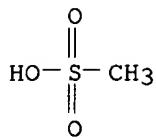


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, 2-(diethylamino)-2-oxoethyl ester, monomethanesulfonate (9CI)  
MF C23 H28 N4 O5 . C H4 O3 S

CM 1

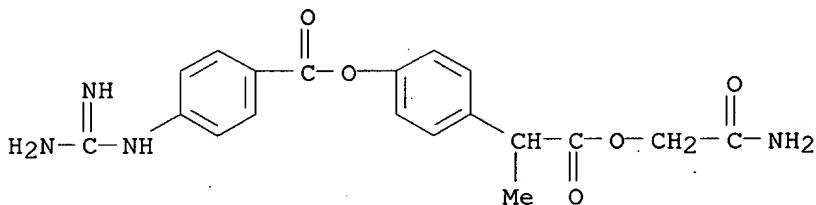


CM 2

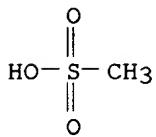


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-methyl-, 2-amino-2-oxoethyl ester, monomethanesulfonate (9CI)  
 MF C19 H20 N4 O5 . C H4 O3 S

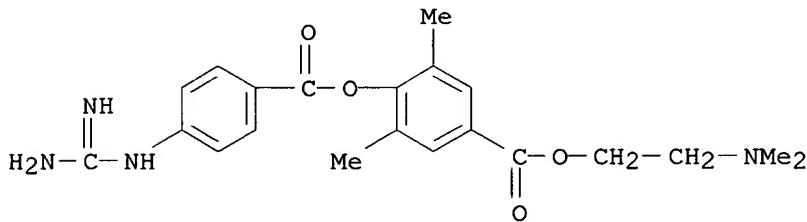
CM 1



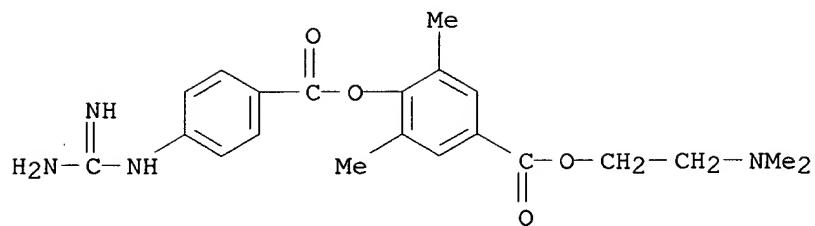
CM 2



L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-3,5-dimethyl-, 2-(dimethylamino)ethyl ester, dihydrochloride (9CI)  
 MF C21 H26 N4 O4 . 2 Cl H



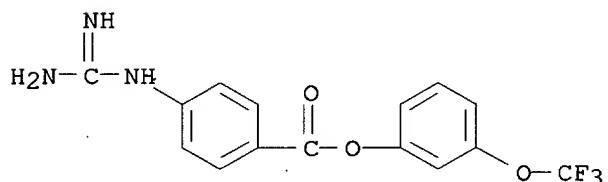
●2 HCl



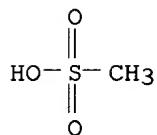
● 2 HCl

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 3-(trifluoromethoxy)phenyl ester, monomethanesulfonate (9CI)  
 MF C15 H12 F3 N3 O3 . C H4 O3 S

CM 1

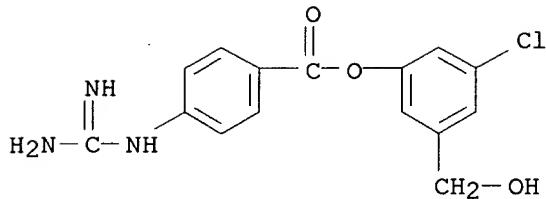


CM 2

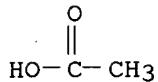


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 3-chloro-5-(hydroxymethyl)phenyl ester, monoacetate (salt) (9CI)  
 MF C15 H14 Cl N3 O3 . C2 H4 O2

CM 1

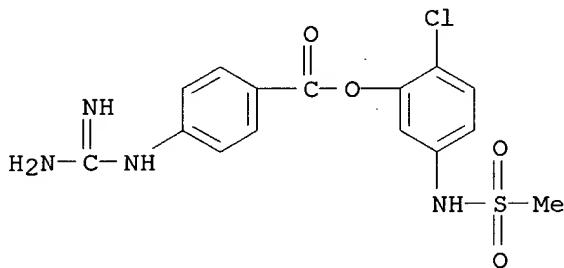


CM 2

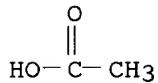


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2-chloro-5-  
 [(methylsulfonyl)amino]phenyl ester, monoacetate (9CI)  
 MF C15 H15 Cl N4 O4 S . C2 H4 O2

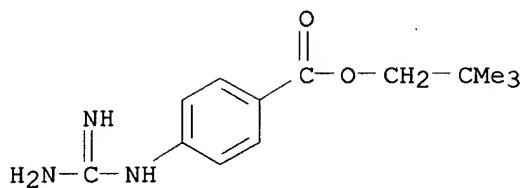
CM 1



CM 2



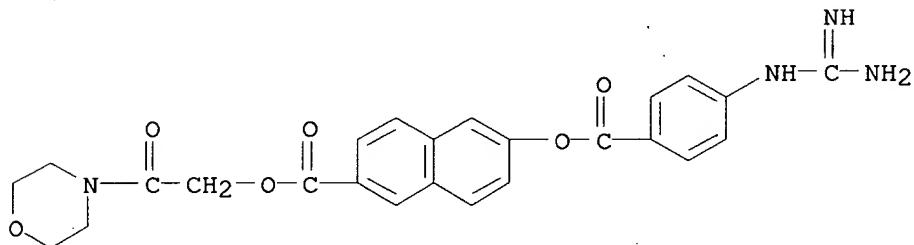
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2,2-dimethylpropyl ester  
 (9CI)  
 MF C13 H19 N3 O2



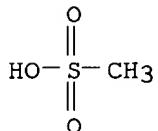
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 2-Naphthalenecarboxylic acid,  
 6-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-  
 , 2-(4-morpholinyl)-2-oxoethyl ester, monomethanesulfonate (9CI)  
 MF C25 H24 N4 O6 . C H4 O3 S

CM 1

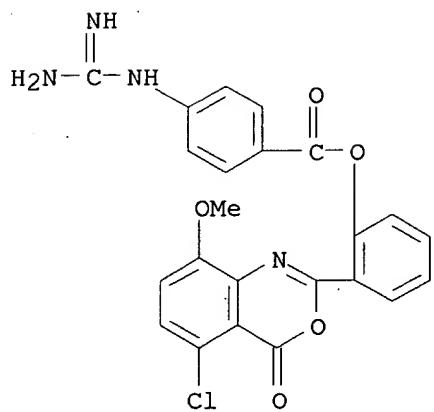


CM 2

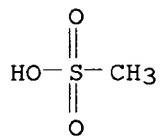


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-,  
 2-(5-chloro-8-methoxy-4-oxo-4H-  
 3,1-benzoxazin-2-yl)phenyl ester, monomethanesulfonate (9CI)  
 MF C23 H17 Cl N4 O5 . C H4 O3 S

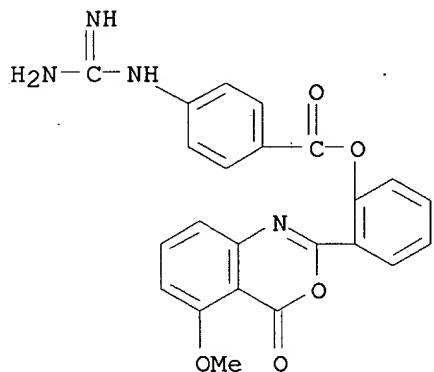
CM 1



CM 2

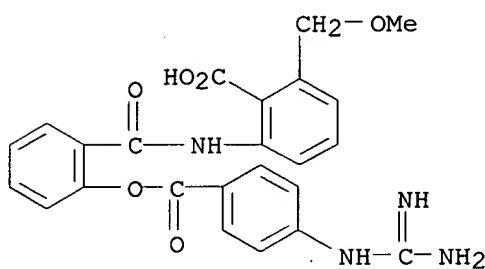


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2-(5-methoxy-4-oxo-4H-3,1-benzoxazin-2-yl)phenyl ester (9CI)  
 MF C23 H18 N4 O5  
 CI COM



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

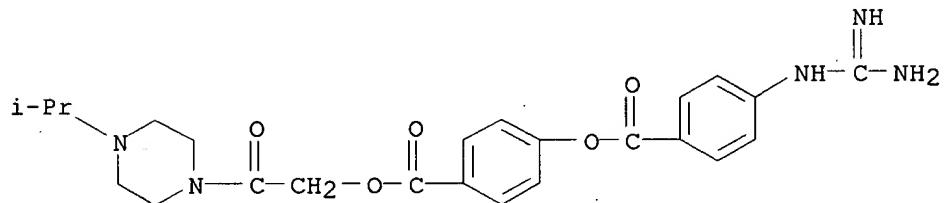
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid,  
 2-[[2-[(4-[(aminoiminomethyl)amino]benzoyl)oxy]benzoyl]amino]  
 ]-6-(methoxymethyl)- (9CI)  
 MF C24 H22 N4 O6  
 CI COM



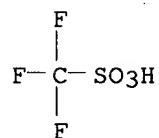
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[2-[4-(1-methylethyl)-1-piperazinyl]-2-oxoethoxy]carbonyl]phenyl ester,  
 mono(trifluoromethanesulfonate) (9CI)  
 MF C24 H29 N5 O5 . C H F3 O3 S

CM 1

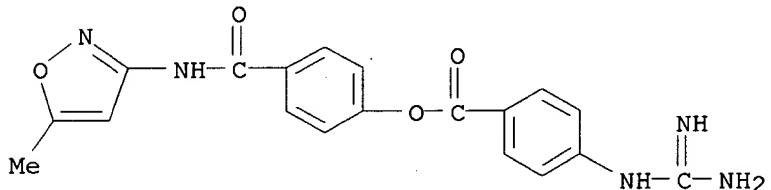


CM 2

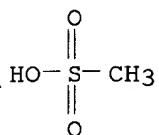


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[5-methyl-3-isoxazolyl]amino]carbonylphenyl ester, monomethanesulfonate (9CI)  
MF C19 H17 N5 O4 . C H4 O3 S

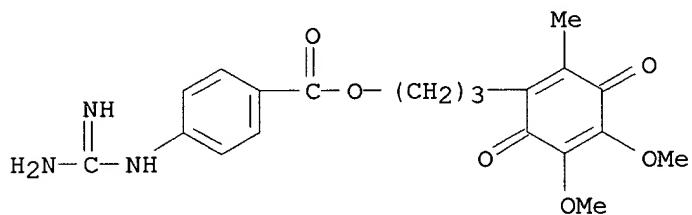
CM 1



CM 2



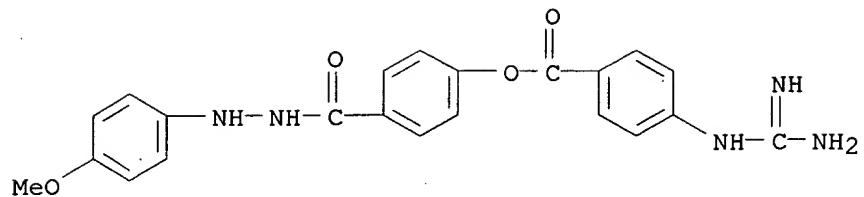
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-,  
3-(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)propyl ester (9CI)  
MF C20 H23 N3 O6



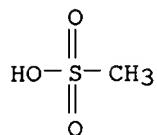
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[[2-(4-methoxyphenyl)hydrazino]carbonylphenyl ester, monomethanesulfonate (9CI)  
MF C22 H21 N5 O4 . C H4 O3 S

CM 1

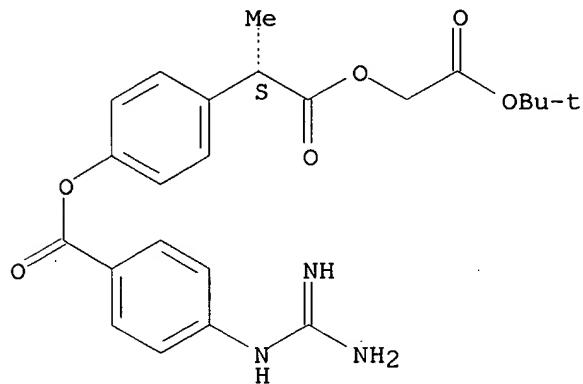


CM 2



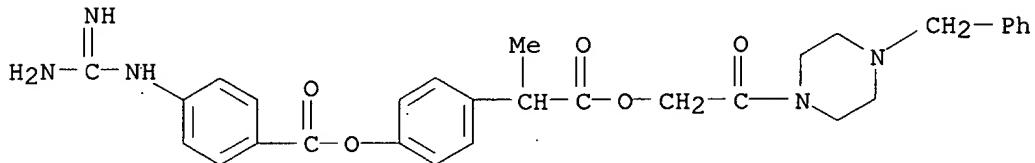
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-  
methyl-, 2-(1,1-dimethylethoxy)-2-oxoethyl ester, (S)- (9CI)  
MF C23 H27 N3 O6  
CI COM

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

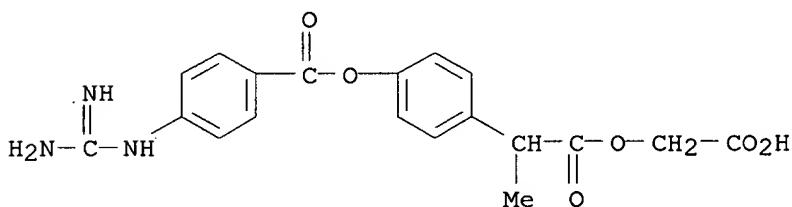
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-  
     methyl-, 2-oxo-2-[4-(phenylmethyl)-1-piperazinyl]ethyl ester (9CI)  
 MF C30 H33 N5 O5  
 CI COM



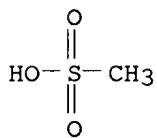
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-  
     methyl-, carboxymethyl ester, monomethanesulfonate (9CI)  
 MF C19 H19 N3 O6 . C H4 O3 S

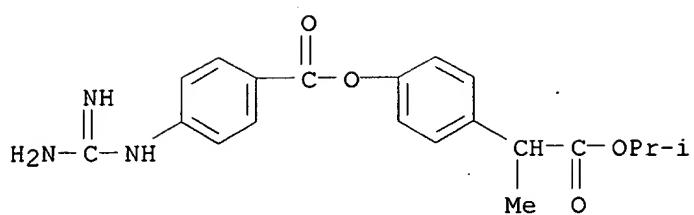
CM 1



CM 2



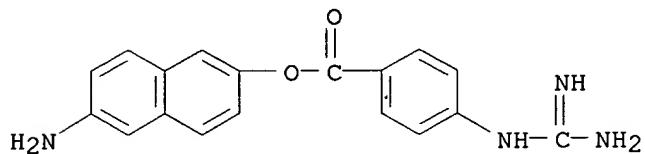
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-.alpha.-  
     methyl-, 1-methylethyl ester (9CI)  
 MF C20 H23 N3 O4  
 CI COM



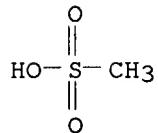
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 6-amino-2-naphthalenyl ester,  
 dimethanesulfonate (9CI)  
 MF C18 H16 N4 O2 . 2 C H4 O3 S

CM 1



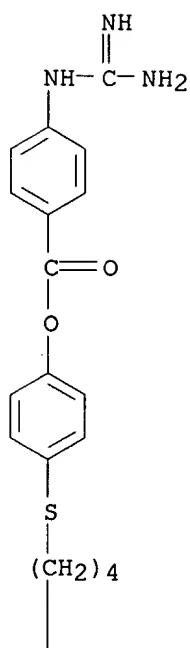
CM 2



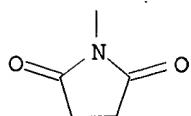
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[(4-(2,5-dioxo-1-pyrrolidinyl)butyl)thio]phenyl ester, monomethanesulfonate (9CI)  
 MF C22 H24 N4 O4 S . C H4 O3 S

CM 1

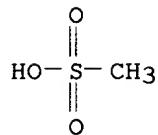
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PAGE 2-A



CM 2

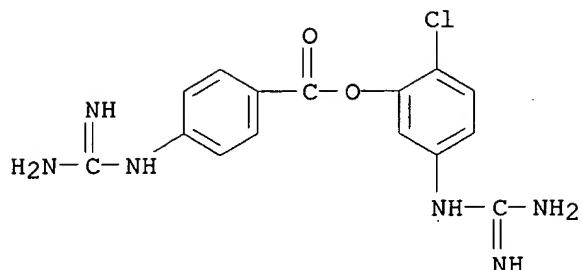


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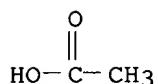
L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-,  
5-[(aminoiminomethyl)amino]-2-  
chlorophenyl ester, diacetate (9CI)

MF C15 H15 Cl N6 O2 . 2 C2 H4 O2

CM 1



CM 2

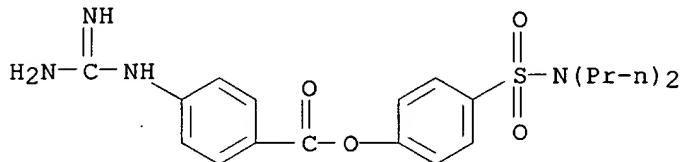


L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS

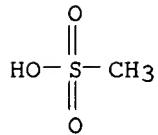
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[  
[(dipropylamino)sulfonyl]phenyl ester, monomethanesulfonate (9CI)

MF C20 H26 N4 O4 S . C H4 O3 S

CM 1

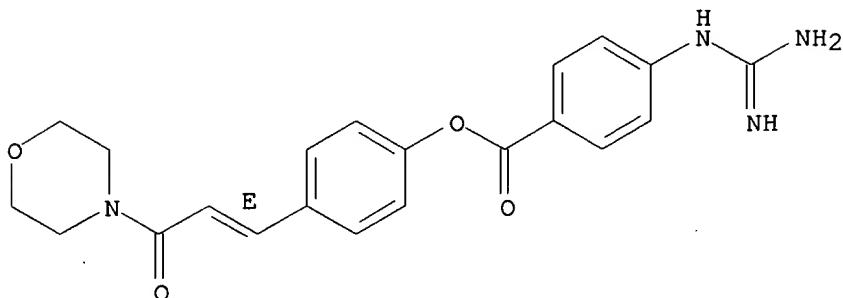


CM 2



L2 50 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 4-[(1E)-3-(4-morpholinyl)-3-oxo-1-propenyl]phenyl ester (9CI)  
MF C21 H22 N4 O4  
CI COM

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):  
'O' IS NOT VALID HERE

To display more answers, enter the number of answers you would like to see. To end the display, enter "NONE", "N", "0", or "END".  
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> search 11 sss full  
FULL SEARCH INITIATED 12:34:48 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 3885 TO ITERATE

100.0% PROCESSED 3885 ITERATIONS 1258 ANSWERS  
SEARCH TIME: 00.00.01

L3 1258 SEA SSS FUL L1

=> file caplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 149.75 149.96

FILE 'CAPLUS' ENTERED AT 12:34:57 ON 03 JUN 2003  
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FILE COVERS 1907 - 3 Jun 2003 VOL 138 ISS 23  
FILE LAST UPDATED: 2 Jun 2003 (20030602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 13  
L4 876 L3

=> ?bact?  
L5 613320 ?BACT?

=> 14 and 15  
L6 31 L4 AND L5

=> d 16 20-31 ti

L6 ANSWER 20 OF 31 CAPLUS COPYRIGHT 2003 ACS  
TI Probiotics: antistaphylococcal activity of 4-aminocyclohexanecarboxylic acid, aminobenzoic acid, and their derivatives and structure-activity relations

L6 ANSWER 21 OF 31 CAPLUS COPYRIGHT 2003 ACS  
TI Cephalosporin compounds

L6 ANSWER 22 OF 31 CAPLUS COPYRIGHT 2003 ACS  
TI The protease inhibitor p-nitrophenyl-p'-guanidinobenzoate inactivates Sindbis and other enveloped viruses

L6 ANSWER 23 OF 31 CAPLUS COPYRIGHT 2003 ACS  
TI 6-[.alpha.-(.omega.-Guanidinoalkanoylamido)acylamido]penicillanic acids

L6 ANSWER 24 OF 31 CAPLUS COPYRIGHT 2003 ACS  
TI 6-[.alpha.-(.omega.-Guanidinoalkanoylamido)acylamido]penicillanic acids

L6 ANSWER 25 OF 31 CAPLUS COPYRIGHT 2003 ACS  
TI Influence of various proteinase inhibitors on the gelatinolytic effect of ejaculated and uterine boar spermatozoa

L6 ANSWER 26 OF 31 CAPLUS COPYRIGHT 2003 ACS  
TI Pharmaceutical cephalosporins

L6 ANSWER 27 OF 31 CAPLUS COPYRIGHT 2003 ACS  
TI Antimicrobial and hypoglycemic (2-imidazolidinylidene)- and (hexahydro-2-pyrimidinylidene)guanidines

L6 ANSWER 28 OF 31 CAPLUS COPYRIGHT 2003 ACS  
TI Specificity and mechanism of clostripain catalysis

L6 ANSWER 29 OF 31 CAPLUS COPYRIGHT 2003 ACS  
TI Antibacterial guanidinoarylpenicillins

L6 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2003 ACS  
TI Tuberculostatic activity of derivatives of aminoguanidine and diaminoguanidine and its correlation with chemical structure

L6 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2003 ACS  
TI Reaction of cyanoguanidine with aromatic amines. II. Formation of 1-amidino-3-(p-nitrophenyl- and p-carboxyphenyl)urea

=> pylori

7936 PYLORI  
20 PYLORIS

L7 7949 PYLORI  
(PYLORI OR PYLORIS)

=> 14 and 17

L8 2 L4 AND L7

=> d 18 1-2 ti

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS  
TI Preparation of esters of 4-guanidinyl(methyl)benzoic acid treating or preventing bacterial infection

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS  
TI Enzyme inhibitors for treatment of gastrointestinal disorders caused by **Helicobacter pylori**

=> d 18 1-2 ti fbib abs

L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS  
TI Preparation of esters of 4-guanidinyl(methyl)benzoic acid treating or preventing bacterial infection

AN 2003:282526 CAPLUS

DN 138:304065

TI Preparation of esters of 4-guanidinyl(methyl)benzoic acid treating or preventing bacterial infection

IN Zhu, Dexu; Muramatsu, Mutsumi; Xie, Jianshu; Cheng, Ni; Wang, Mingwei

PA Peop. Rep. China

SO PCT Int. Appl., 43 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

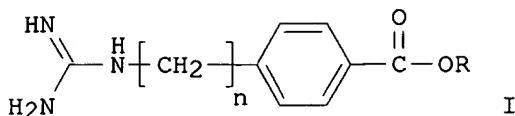
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PI	WO 2003029201	A1	20030410	WO 2001-CN1499	20011023	
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

CN 1410419

A 20030416

CN 2001-142289 A 20010926  
CN 2001-142289 20010926

GI



AB Title compds. I [n = 0-1; R = H, alkyl, aryl, biphenyl deriv.] are prep'd. For instance, a suspension of 4-guanidinomethylbenzoic acid hydrochloride (prepn. given) is condensed with phenol (pyridine, DCC, 48 h) to give Ph 4-guanidinomethylbenzoate hydrochloride. Selected analogs had IC50 of >200 - 26 .mu.M on E. coli growth. Another example compd. had MIC of

0.10

- 0.48 .mu.g/mL against 9 strains of *H. pylori* at various pH. I are useful for treating or preventing disease or disorders caused by or assoc'd. with certain bacterial infection, esp. *Escherichia coli* (*E. coli*) or *Helicobacter pylori* (*H. pylori*) infection.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS  
TI Enzyme inhibitors for treatment of gastrointestinal disorders caused by *Helicobacter pylori*  
AN 1994:587325 CAPLUS  
DN 121:187325  
TI Enzyme inhibitors for treatment of gastrointestinal disorders caused by *Helicobacter pylori*  
IN Wabnitz, Rudolf; Riedl, Jutta; Ansorg, Rainer; Goebell, Harald  
PA Asche AG, Germany  
SO Ger. Offen., 3 pp.  
CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 4305536	A1	19940825	DE 1993-4305536	19930219
	WO 9418964	A1	19940901	WO 1994-EP523	19940218
	W: AU, CA, FI, HU, JP, NO, US RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE			DE 1993-4305536A	19930219
	AU 9462053	A1	19940914	AU 1994-62053	19940218
				DE 1993-4305536A	19930219
				WO 1994-EP523	W 19940218
	EP 804184	A1	19971105	EP 1994-909036	19940218
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE			DE 1993-4305536A	19930219
	JP 2002515002	T2	20020521	WO 1994-EP523	W 19940218
				JP 1994-518670	19940218
				DE 1993-4305536A	19930219
	WO 9614068	A1	19960517	WO 1994-EP523	W 19940218
				WO 1994-EP3669	19941107

W: AT, CA, FI, HU, JP, NO, US  
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE  
DE 1993-4305536 19930219

AB Enzyme inhibitors, esp. protease inhibitors such as .omega.-guanidinocarboxylic acid esters, are useful for treatment of *H. pylori*-assocd. gastrointestinal disorders. Thus, soft gelatin capsules contained camostat 100.00, soybean lecithin 5.00, 2,6-di-tert-butyl-4-methylphenol (antioxidant) 0.1, and peanut oil to 800.00 mg.

=> d 18 2 it

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS  
IT Carboxylic acids, biological studies  
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(guanidino, esters, Helicobacter *pylori*-assocd. digestive disorder treatment with)  
IT Campylobacter *pyloridis*  
(infection with, digestive disorder from, treatment of, with proteinase inhibitors)  
IT Enzymes  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(inhibitors, Helicobacter *pylori*-assocd. digestive disorder treatment with)  
IT Digestive tract  
(disease, infection, with Helicobacter *pylori*, treatment of, with proteinase inhibitors)  
IT Onium compounds  
RL: BIOL (Biological study)  
(guanidinium, carboxy, Helicobacter *pylori*-assocd. digestive disorder treatment with)  
IT 6659-35-4D, .epsilon.-Guanidinocaproic acid, esters 16060-65-4D,  
p-Guanidinobenzoic acid, esters 37205-61-1, Proteinase inhibitor  
39492-01-8, Gabexate 59721-28-7, Camostat 71079-09-9,  
FOY 251 81525-10-2, Nafamostat  
RL: BIOL (Biological study)  
(Helicobacter *pylori*-assocd. digestive disorder treatment with)

=> 59721-28-7

**REGISTRY INITIATED**

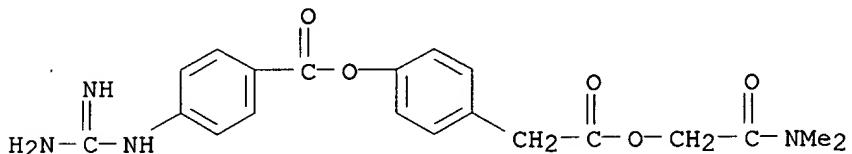
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Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

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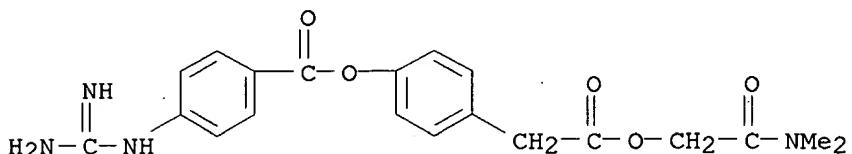
82 L9

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ENTER ANSWER NUMBER OR RANGE (1):1-5

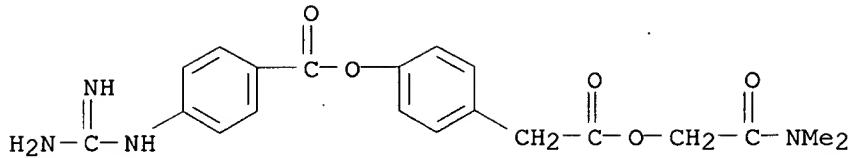
L10 ANSWER 1 OF 82 CAPLUS COPYRIGHT 2003 ACS  
 IT 59721-28-7, Camostat  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
     (development of camostat mesilate troche for prevention of mucositis  
     in  
         mouth during cancer chemotherapy (Erratum))  
 RN 59721-28-7 CAPLUS  
 CN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-,  
     2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



L10 ANSWER 2 OF 82 CAPLUS COPYRIGHT 2003 ACS  
 IT 59721-28-7, Camostat  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
     (Biological study); USES (Uses)  
     (trypsin inhibitor camostat has different effects on pancreas between  
     cholecystokinin-A receptor gene knockout and wild-type mice)  
 RN 59721-28-7 CAPLUS  
 CN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-,  
     2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



L10 ANSWER 3 OF 82 CAPLUS COPYRIGHT 2003 ACS  
 IT 59721-28-7, Camostat  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
     (metabolite; development of camostat mesilate troche for prevention of  
     mucositis in mouth during cancer chemotherapy)  
 RN 59721-28-7 CAPLUS  
 CN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-,  
     2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



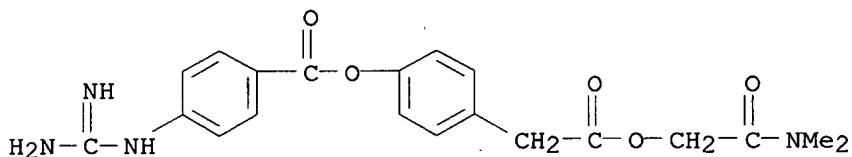
L10 ANSWER 4 OF 82 CAPLUS COPYRIGHT 2003 ACS

IT **59721-28-7**

RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)  
(fish feed contg. proteinase inhibitors)

RN 59721-28-7 CAPLUS

CN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-,  
2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



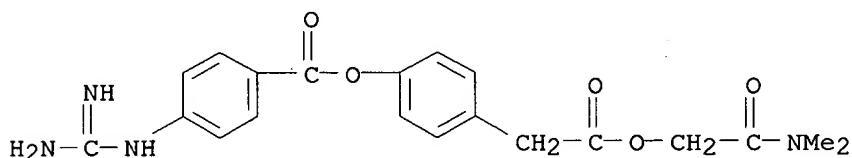
L10 ANSWER 5 OF 82 CAPLUS COPYRIGHT 2003 ACS

IT **59721-28-7, Camostat**

RL: PEP (Physical, engineering or chemical process); PRP (Properties);  
THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)  
(prepn. and characterization of biodegradable or enteric-coated  
microspheres contg. the protease inhibitor camostat)

RN 59721-28-7 CAPLUS

CN Benzeneacetic acid, 4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]-,  
2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



=> logoff hold

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE

ENTRY

13.16

TOTAL

SESSION

179.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

CA SUBSCRIBER PRICE

ENTRY	SESSION
0.00	-1.30

SESSION WILL BE HELD FOR 60 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 12:40:34 ON 03 JUN 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1623paz

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
SESSION RESUMED IN FILE 'CAPLUS' AT 12:42:25 ON 03 JUN 2003  
FILE 'CAPLUS' ENTERED AT 12:42:25 ON 03 JUN 2003  
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	13.16	179.28
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.30

=> file reg	COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST		13.58	179.70
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)		SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE		0.00	-1.30

FILE 'REGISTRY' ENTERED AT 12:42:50 ON 03 JUN 2003  
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STRUCTURE FILE UPDATES: 1 JUN 2003 HIGHEST RN 523977-56-2  
DICTIONARY FILE UPDATES: 1 JUN 2003 HIGHEST RN 523977-56-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

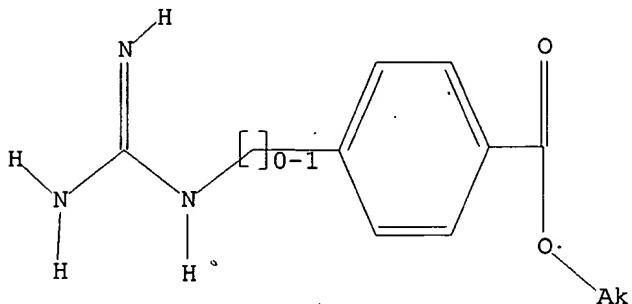
Experimental and calculated property data are now available. See HELP  
PROPERTIES for more information. See STNote 27, Searching Properties

in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>  
Uploading 09975136 before allowance.str

L11       STRUCTURE UPLOADED

=> d l11  
L11 HAS NO ANSWERS  
L11                   STR



G1 H,Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED -     208 TO ITERATE

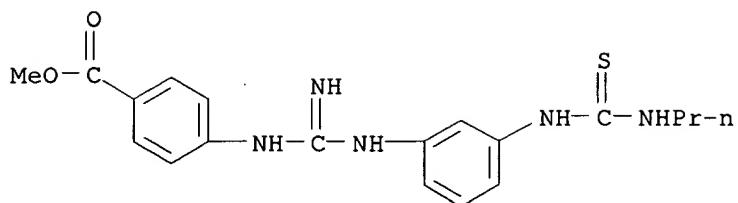
100.0% PROCESSED     208 ITERATIONS                           9 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:   ONLINE    \*\*COMPLETE\*\*  
                                 BATCH    \*\*COMPLETE\*\*  
PROJECTED ITERATIONS:      3295 TO    5025  
PROJECTED ANSWERS:         9 TO      360

L12        9 SEA SSS SAM L11

=> d scan

L12 9 ANSWERS    REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, p-[3-[m-(3-propyl-2-thioureido)phenyl]guanidino]-, methyl  
ester, monohydrochloride (8CI)  
MF C19 H23 N5 O2 S . Cl H



HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>

=>

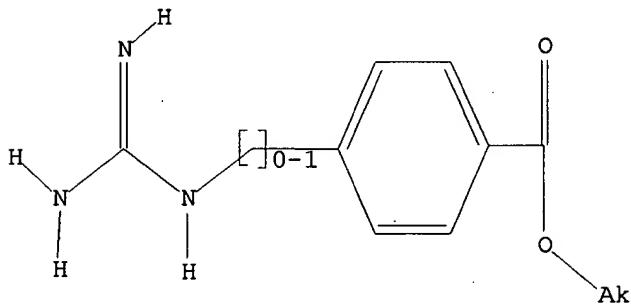
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L13        STRUCTURE UPLOADED

=> d 113

L13 HAS NO ANSWERS

L13                    STR



G1 H,Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

=> search l13 sss sam

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SAMPLE SCREEN SEARCH COMPLETED -     208 TO ITERATE

100.0% PROCESSED      208 ITERATIONS  
SEARCH TIME: 00.00.01

9 ANSWERS

FULL FILE PROJECTIONS: ONLINE    \*\*COMPLETE\*\*

BATCH        \*\*COMPLETE\*\*

PROJECTED ITERATIONS:      3295 TO      5025

PROJECTED ANSWERS:            9 TO      360

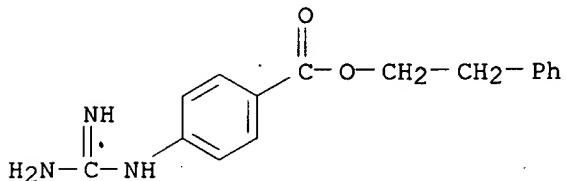
L14

9 SEA SSS SAM L13

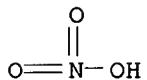
=> d scan

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2-phenylethyl ester,  
mononitrate (9CI)  
MF C16 H17 N3 O2 . H N O3

CM 1



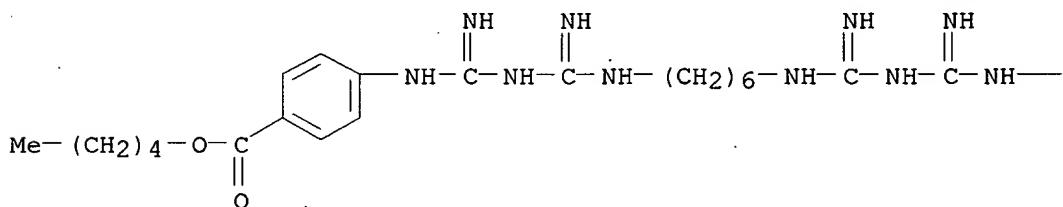
CM 2



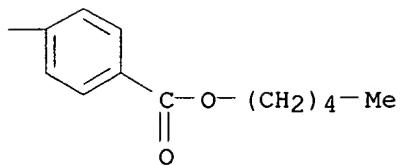
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):8

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4,4'-(1,3,12,14-tetraimino-2,4,11,13-tetraazatetradecane-1,14-diyl)diimino]bis-, dipentyl ester, dihydrochloride (9CI)  
MF C34 H52 N10 O4 . 2 Cl H

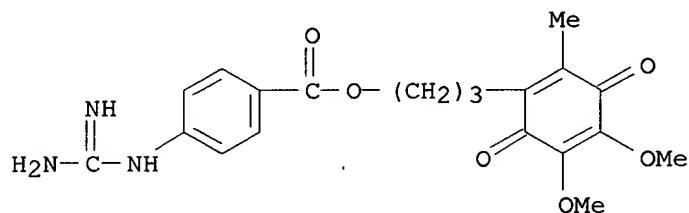
PAGE 1-A



●2 HCl

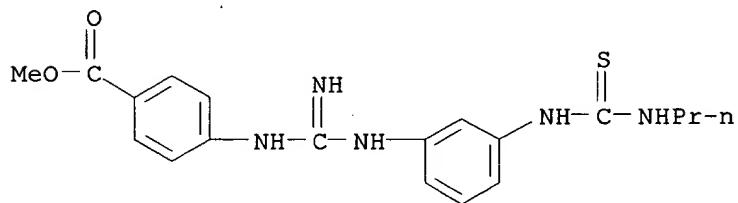


L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[(aminoiminomethyl)amino]-,  
 3-(4,5-dimethoxy-2-methyl-3,6-  
 dioxo-1,4-cyclohexadien-1-yl)propyl ester (9CI)  
 MF C20 H23 N3 O6



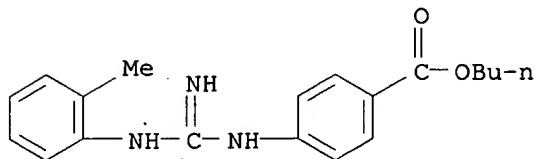
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, p-[3-[(3-propyl-2-thioureido)phenyl]guanidino]-, methyl  
 ester, monohydrochloride (8CI)  
 MF C19 H23 N5 O2 S . Cl H



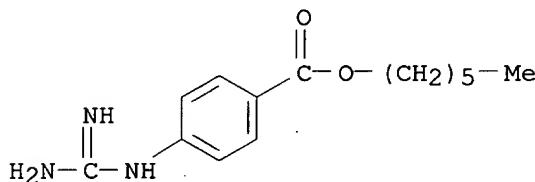
HCl

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[[imino[(2-methylphenyl)amino]methyl]amino]-, butyl ester  
(9CI)  
MF C19 H23 N3 O2



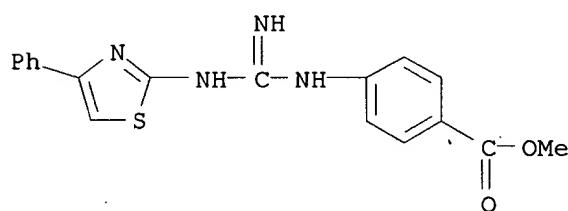
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, hexyl ester (9CI)  
MF C14 H21 N3 O2  
CI COM



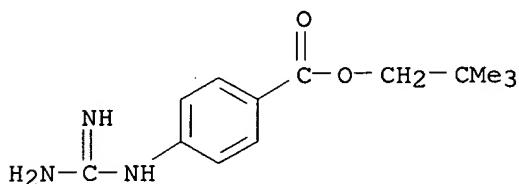
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[[imino[(4-phenyl-2-thiazolyl)amino]methyl]amino]-,  
methyl  
ester (9CI)  
MF C18 H16 N4 O2 S



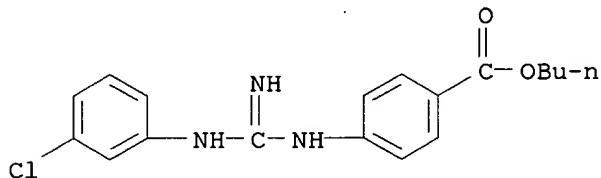
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2,2-dimethylpropyl ester  
(9CI)  
MF C13 H19 N3 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L14 9 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[[[(3-chlorophenyl)amino]iminomethyl]amino]-, butyl ester  
(9CI).  
MF C18 H20 Cl N3 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> e Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2,2-dimethylpropyl ester/cn  
E1 1 BENZOIC ACID,  
4,6-DIMETHOXY-3-(5-METHOXY-2-(METHOXCARBONYL)  
-3-PENTYLPHENOXY)-2-PENTYL-, METHYL ESTER/CN  
E2 1 BENZOIC ACID, 4,6-DIMETHOXY-3-METHYL-2-(1-OXOBUTOXY)-,  
METHY  
L ESTER/CN  
E3 0 --> BENZOIC ACID, 4-(AMINOIMINOMETHYL)AMINO-, 2,2-DIMETHYLPROP  
YL ESTER/CN  
E4 1 BENZOIC ACID,  
4-(((((2,3-DIHYDRO-2,2-DIMETHYL-7-BENZOFURA

NYL) OXY) CARBONYL) METHYLAMINO) CARBONYL) AMINO) SULFONYL) AMINO) -  
                          , ETHYL ESTER/CN  
 E5                  1  BENZOIC ACID,  
 4-((((((2,3,4-TRICHLOROPHENYL) THIO) ACETYL) OXY  
                          ) ACETYL) AMINO) METHYL) -, METHYL ESTER/CN  
 E6                  1  BENZOIC ACID,  
 4-((((((3.BETA.)-17-OXOANDROST-5-EN-3-YL) AMIN  
                          O) CARBONYL) OXY) METHYL) AMINO) -, 2-(DIETHYLA  
 ESTER/C  
                          N  
 E7                  1  BENZOIC ACID,  
 4-((((((3.BETA.)-17-OXOANDROST-5-EN-3-YL) OXY  
                          METHYL) THIO) METHYL) AMINO) -, 2-(DIMETHYLA  
 ESTER/CN  
 E8                  1  BENZOIC ACID,  
 4-((((((3.BETA.,17.BETA.)-3-HYDROXYANDROST-5-  
                          EN-17-YL) AMINO) CARBONYL) OXY) METHYL) AMINO) -,  
 2-(DIETHYLA  
                          N  
 E9                  1  BENZOIC ACID,  
 4-((((((4-BROMO-8-CHLORO-1-NAPHTHALENYL) THIO)  
                          ACETYL) OXY) ACETYL) AMINO) METHYL) -, METHYL ESTER/CN  
 E10                1  BENZOIC ACID,  
 4-((((((4-CHLOROPHENYL) AMINO) CARBONYL) HYDRAZO  
                          NO) PHENYLMETHYL) THIO) METHYL) -, 1,1-DIMETHYLETHYL ESTER/CN  
 E11                1  BENZOIC ACID,  
 4-((((((4-CHLOROPHENYL) SULFONYL) AMINO) PHENYLM  
                          ETHYLENE) AMINO) THIOMETHYL) AMINO) -/CN  
 E12                1  BENZOIC ACID,  
 4-((((((4-METHOXYPHENYL) SULFONYL) (PHENYLMETHY  
                          L) AMINO) ACETYL) AMINO) OXY) DIPHENYLMETHYL) -/CN  
  
 => e Benzoic acid, 4-((aminoiminomethyl)amino) -, 2,2-dimethylpropyl ester/cn  
 E1                1  BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -, 1-NAPHTHALENYL  
 E  
                          STER, METHANESULFONATE/CN  
 E2                1  BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -, 1-NAPHTHALENYL  
 E  
                          STER, MONONITRATE/CN  
 E3                1 --> BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -,  
 2,2-DIMETHYLPROP  
                          YL ESTER/CN  
 E4                1  BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -,  
 2,3-DIFLUOROPHEN  
                          YL ESTER/CN  
 E5                1  BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -,  
 2,3-DIFLUOROPHEN  
                          YL ESTER, MONOACETATE/CN  
 E6                1  BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -,  
 2,3-DIMETHOXYPHE  
                          NYL ESTER, MONOHYDROCHLORIDE/CN  
 E7                1  BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -,  
 2,3-DIMETHYLPHEN  
                          YL ESTER/CN  
 E8                1  BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -,  
 2,3-DIMETHYLPHEN  
                          YL ESTER, MONOMETHANESULFONATE/CN  
 E9                1  BENZOIC ACID, 4-((AMINOIMINOMETHYL) AMINO) -,  
 2,4-DINITROPHENY

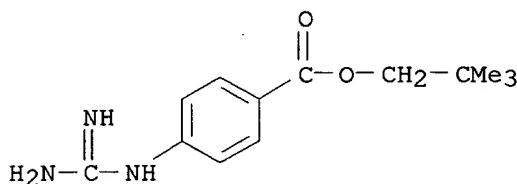
E10 1 L ESTER/CN  
 BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,  
 2,5-DICHLOROPHEN  
 E11 1 YL ESTER/CN  
 BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,  
 2,5-DICHLOROPHEN  
 E12 1 YL ESTER, MONOMETHANESULFONATE/CN  
 BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,  
 2,6-DICHLORO-4-N ITROPHENYL ESTER/CN

=> e3

L15 1 "BENZOIC ACID, 4-((AMINOIMINOMETHYL)AMINO)-,  
 2,2-DIMETHYLPROPYL  
 ESTER"/CN

=> d 115

L15 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS  
 RN 282718-30-3 REGISTRY  
 CN Benzoic acid, 4-[(aminoiminomethyl)amino]-, 2,2-dimethylpropyl ester  
 (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C13 H19 N3 O2  
 SR CA  
 LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

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		0.00	-1.30

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FILE LAST UPDATED: 2 Jun 2003 (20030602/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> l15
L16      1 L15

=> d 116 ti fbib abs

L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS
TI (4-aminomethyl)phenylguanidine derivatives as nonpeptidic highly
selective
    inhibitors of human urokinase
AN 2000:341443 CAPLUS
DN 133:99075
TI (4-aminomethyl)phenylguanidine derivatives as nonpeptidic highly
selective
    inhibitors of human urokinase
AU Sperl, Stefan; Jacob, Uwe; De Prada, Nuria Arroyo; Sturzebecher, Jorg;
    Wilhelm, Olaf G.; Bode, Wolfram; Magdolen, Viktor; Huber, Robert;
    Moroder,
    Luis
CS Max-Planck-Institut fur Biochemie, Martinsried, 82152, Germany
SO Proceedings of the National Academy of Sciences of the United States of
    America (2000), 97(10), 5113-5118
    CODEN: PNASA6; ISSN: 0027-8424
PB National Academy of Sciences
DT Journal
LA English
AB Increased expression of the serine protease urokinase-type plasminogen
activator (uPA) in tumor tissues is highly correlated with tumor cell
migration, invasion, proliferation, progression, and metastasis. Thus
inhibition of uPA activity represents a promising target for
antimetastatic therapy. So far, only the x-ray crystal structure of uPA
inactivated by H-Glu-Gly-Arg-chloromethylketone has been reported, thus
limited data are available for a rational structure-based design of uPA
inhibitors. Taking into account the trypsin-like arginine specificity of
uPA, (4-aminomethyl)phenylguanidine was selected as a potential P1
residue
    and iterative derivatization of its amino group with various hydrophobic
    residues, and structure-activity relationship-based optimization of the
    spacer in terms of hydrogen bond acceptor/donor properties led to
    N-(1-adamantyl)-N'-(4-guanidinobenzyl)urea as a highly selective
```

nonpeptidic uPA inhibitor. The x-ray crystal structure of the uPA B-chain

complexed with this inhibitor revealed a surprising binding mode consisting of the expected insertion of the phenylguanidine moiety into the S1 pocket, but with the adamantyl residue protruding toward the hydrophobic S1' enzyme subsite, thus exposing the ureido group to hydrogen-bonding interactions. Although in this enzyme-bound state the inhibitor is crossing the active site, interactions with the catalytic residues Ser-195 and His-57 are not obsd., but their side chains are spatially displaced for steric reasons. Compared with other trypsin-like serine proteases, the S2 and S3/S4 pockets of uPA are reduced in size because of the 99-insertion loop. Therefore, the peculiar binding mode

of

the new type of uPA inhibitors offers the possibility of exploiting optimized interactions at the S1'/S2' subsites to further enhance selectivity and potency. Because crystals of the uPA/benzamidine complex allow inhibitor exchange by soaking procedures, the structure-based design

of new generations of uPA inhibitors can rely on the assistance of x-ray anal.

RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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CA SUBSCRIBER PRICE	-0.65	-1.95	

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NEWS 17 Dec 17 TOXCENTER enhanced with additional content  
NEWS 18 Dec 17 Adis Clinical Trials Insight now available on STN  
NEWS 19 Jan 29 Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC  
NEWS 20 Feb 13 CANCERLIT is no longer being updated  
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NEWS 22 Feb 24 PCTGEN now available on STN  
NEWS 23 Feb 24 TEMA now available on STN  
NEWS 24 Feb 26 NTIS now allows simultaneous left and right truncation  
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NEWS 26 Mar 04 SDI PACKAGE for monthly delivery of multifile SDI results  
NEWS 27 Mar 20 EVENTLINE will be removed from STN  
NEWS 28 Mar 24 PATDPAFULL now available on STN  
NEWS 29 Mar 24 Additional information for trade-named substances without structures available in REGISTRY  
NEWS 30 Apr 11 Display formats in DGENE enhanced  
NEWS 31 Apr 14 MEDLINE Reload  
NEWS 32 Apr 17 Polymer searching in REGISTRY enhanced  
NEWS 33 Apr 21 Indexing from 1947 to 1956 being added to records in CA/CAPLUS  
NEWS 34 Apr 21 New current-awareness alert (SDI) frequency in WPIDS/WPINDEX/WPIX  
NEWS 35 Apr 28 RDISCLOSURE now available on STN  
NEWS 36 May 05 Pharmacokinetic information and systematic chemical names added to PHAR  
NEWS 37 May 15 MEDLINE file segment of TOXCENTER reloaded  
NEWS 38 May 15 Supporter information for ENCOMPPAT and ENCOMPLIT updated  
NEWS 39 May 16 CHEMREACT will be removed from STN  
NEWS 40 May 19 Simultaneous left and right truncation added to WSCA  
NEWS 41 May 19 RAPRA enhanced with new search field, simultaneous left and right truncation  
NEWS 42 Jun 06 Simultaneous left and right truncation added to CBNB  
NEWS 43 Jun 06 PASCAL enhanced with additional data  
  
NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003  
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